

## **AMENDMENTS TO THE DRAWINGS**

Please replace all 29 of the original drawings sheets with the enclosed 29 replacement sheets.

## **REMARKS**

The following remarks and the above amendments are submitted to address all issues in this case, and to put this case in condition for allowance. Applicant replaces the prior claims with a new claim simply to better define the subject matter of the present invention; no new matter is added by the new claim and the subject matter of the new claim is supported by the original specification, as filed. After the above amendment, application claim 12 is the only claim pending in the application. Application claim 12 is the only independent claim.

Applicant has studied the Office Action mailed October 12, 2006, and has the following remarks.

### **Oath/Declaration**

Submitted with this Response is a declaration incorporating the initial change that has been executed by inventor William Welsh. Applicant believes this declaration, in conjunction with the originally filed declaration, should resolve the concerns of the Examiner.

### **Drawings**

Submitted with this Response are replacement drawing sheets labeled in compliance with 37 CFR 1.121(d) to replace the present sheets of the drawings. It is believed that these sheets should resolve all the outstanding issues related to labeling of the drawing sheets.

### **Specification**

The Examiner objected to the use of the trademark "CoMFA" in the disclosure. To try and resolve the Examiner's concerns, Applicants have amended the specification to present the CoMFA trademark in capitals and identify the generic name of the product.

The Examiner also contended that the abstract, as submitted, referred to purported merits of the invention and provided “methods and systems,” while the claims are solely directed to methods. While Applicant would contend that the application includes systems, the abstract has been amended in a fashion which is believed to rectify the Examiner’s concerns.

These amendments to the specification are believed to be supported by the disclosure of the specification as initially filed and are, therefore, not believed to comprise new matter.

### **35 U.S.C. § 101**

The Examiner rejected claims 1-11 under 35 U.S.C. § 101 as being directed to non-statutory subject matter. Without admission as to the correctness of this rejection, claims 1-11 have been cancelled in favor of claim 12.

New claim 12 specifically recites that a distribution indicative of molecular shape is stored for comparison to other distributions related to other molecular shapes. The Examiner contended that the prior claims failed under § 101 for not producing a tangible result, based on the Examiner’s apparent belief that the method as claimed “may take place entirely within the confines of a computer or a human mind without any communication to the outside world.”

Applicant respectfully contends that the method described in new claim 12 produces a tangible result. Specifically, the method produces a distribution which is indicative of shape, and stores that distribution for later comparison to distributions indicative of shape for other molecules.

The tangibility requirement effectively only requires that the claim recite more than a judicial exception. See Interim Guidelines, p. 20 (“The claim must be examined to see if it includes *anything more* than a § 101 judicial exception.”) (emphasis added). It is believed the Examiner was concerned the process of the prior claims recited only an abstract idea. Applicants

respectfully traverse as claim 12 creates a tangible result in the form of a stored distribution indicative of molecular shape, which can be used for comparison to other molecules' shape. This is a tangible result in that it creates useful data, such as to get a preliminary indication of potential biological effect of a molecule, as discussed in the present application.

### **35 U.S.C. § 112**

The Examiner rejected Claims 1-11 under 35 U.S.C. § 112 as being indefinite for failing to particularly point out and distinctly claim the subject matter of the invention. Without admission as to the correctness of the Examiner's rejection. Claims 1-11 and have cancelled. It is believed by Applicants that new claim 12 meets the requirements of §112.

### **35 U.S.C. § 102**

The Examiner rejected Claims 1-4 and 8-11 as being anticipated by Zauhar et al. (Issues and Applications in Toxicology and Risk Assessment Meeting, April, 2001) and claim 7 as being anticipated by Zauhar et al. (ACS national meeting, August, 1999). Without admission as to the correctness of these rejections, claims 1-11 have been cancelled in favor of new claim 12.

Applicants assert that neither of the cited references serves to anticipate or render obvious the subject matter of new claim 12. New claim 12 specifically indicates that the iterative process of ray segment tracing is stopped prior to recording if a ray segment is determined to simply span a single component atom of the molecule. The process is then continued using the same impact point of the prior ray but with a newly selected direction for the new ray. The process is continued until a fixed number of ray segments have been recorded resulting in the ray trace. As discussed in the instant specification (see, for example, page 19), this segment culling can provide for more meaningful information being encoded by the ray trace.

The cited references appear to be silent on how the ray segments are drawn and specifically fail to show restarting the ray trace in the event that a single ray segment only spans a individual atom.

As the references are required to show all elements in order to anticipate, neither of the cited references can anticipate the new claim. Further, such a stopped and restarted iteration when the ray segment is across an atom does not appear to be contemplated by either reference, and therefore does not appear to render such claim obvious.

### **Conclusion**


In light of the above, Applicants respectfully request entrance of the above amendment and allowance of all pending claims so that this case can pass on to issue.

As a final point, enclosed herewith is a petition for a one month extension of time and the associated petition fee. It is believed no other fees are due in conjunction with this filing; however, the Commissioner is authorized to credit any overpayment or charge any deficiencies necessary for entering this amendment, including any claims fees and/or extension fees to/from our **Deposit Account No. 50-0975**.

If any questions remain, Applicant respectfully requests a telephone call to the below-signed attorney at (314) 444-7783.

Respectfully submitted,

Lewis, Rice & Fingersh, L.C.



---

Kirk A. Damman  
Registration No. 42,461  
Attorney for Applicant

February 12, 2007

Lewis, Rice and Fingersh, L.C.

500 N. Broadway, Suite 2000  
St. Louis, MO 63102-2147  
Tel: (314) 444-7600  
Fax: (314) 444-7788